Updated 12-15-09

CINT Scientist Summaries

George Bachand
Primary research interests are in the area of nano-bio interfaces, materials, and systems, with emphasis on understanding and exploiting active biological molecules as structural and functional components of integrated nanosystems. Interests also include smart materials, bio-mimetic and -inspired manufacturing strategies, biological materials from extremophilic sources, and stochastic, non-equilibrium assembly processes. Current research activities are focused on engineering *in vitro* biological transport systems for (1) driving the active assembly of composite nanomaterials, and (2) transporting biological and synthetic materials in nanofluidic systems and devices. Research includes isolation, modification, and characterization of structural/functional proteins, functionalization strategies to interface synthetic and biological materials, dynamic surface chemistry to regulate biomolecule functionality, and biological molecules as nanoscale scaffolds for hybrid materials assembly. Research skills include gene isolation and cloning, recombinant protein expression and characterization, site-directed mutagenesis, genetic engineering, protein engineering and modification, prokaryotic/eukaryotic cell culture, surface functionalization, and a variety of biochemical and immunological techniques. The primary CINT capabilities utilized include molecular biosynthesis of proteins and DNA-based materials, biochemical/biophysical characterization of proteins, cell culture, and brightfield and epifluorescence microscopy.

Contact: gdbacha@sandia.gov, (505) 844-5164 (*on temporary leave of absence until 2010*)
Thrust: Soft, Biological and Composite Nanomaterials
Location: Core Facility

A.V. (Sasha) Balatsky
Research interests include: noise spectroscopy of extreme quantum systems, single spin detection in tunneling and coupling between electronic and magnetic degrees of freedom in nanoscale devices. I am also interested in effects of impurities, defects, surfaces, interfaces, and other inhomogeneities on local electronic properties, and how they control functionality at nanoscale. Recent specific research includes theory of single impurities in high temperature superconductors; Effects of single spin dynamics on metallic surfaces; Theory of electron tunneling through quantum dots with electron-electron correlation, single molecules with electron-vibration coupling, Inelastic Electron Tunneling Spectroscopy in DNA.

*Contact:*avb@lanl.gov, (505) 665-0077
Thrust: Theory and Simulation of Nanoscale Phenomena
Location: Gateway Facility

Igal Brener
Primary research interests are in the area of nanophotonics, or in other words, optics at subwavelength scales, spanning the visible to the far-infrared, and crossover/applications to other disciplines such as biology, biochemistry and chem-bio sensing. Some specific research topics that we are particularly interested in at the moment are: 1) Nano-plasmonics and optical interactions in nanofabricated metallic structures, using self-assembly, colloidal synthesis or e-beam lithography; examples are surface-enhanced Raman scattering (SERS), localized surface plasmons in metallic nanostructures, nano-antennas and energy transfer and the physics of nanohole arrays. 2) Static and adaptable metamaterials: novel optical phenomena using novel metamaterial designs; 2D and 3D nanofabrication of metamaterials using CINT's tools (optical lithography, e-beam writing, X-ray lithography, etc); energy transfer to biomolecules anchored to surfaces of metamaterial cells. 3) Nanophotonics in silicon/silicon nitride microresonators: ultra high Q optical microresonators and photon-matter interactions on the surfaces of such resonators. 4) Nanophotonics and micro-optics in microfluidic devices that integrate particle manipulation capabilities (dielectrophoresis or ultrasonic manipulation); sub-wavelength imaging and spectroscopy in microfluidics (fluorescence and Raman). 5) Terahertz science: emission, detection, spectroscopy, imaging, and novel devices. Research skills include low temperature PL/Raman and micro-PL, ultrafast nonlinear spectroscopy (nonlinear absorption, four-wave mixing, harmonic generation), a variety of terahertz techniques (TDS, CW, Photomixing), fluorescence microscopy, fabrication of nanostructures, microfluidics and microacoustics using optical lithography and other clean-room techniques. The primary CINT capabilities utilized include cryogenic systems for optical measurements (down to 4K), fluorescent and confocal microscopes, THz-TDS and THz

photomixing systems, Raman and PL spectrometers, laser-diode switching hardware, waveguide coupling systems including fiber pigtailing, microfluidic support equipment, piezoelectric control and ultrasonic measurements.

Contact: ibrener@sandia.gov, (505) 844-8097
Thrust: Nanophotonics and Optical Nanomaterials
Location: Core Facility

Bruce Bunker
Primary research interests involve understanding, manipulating, and exploiting the interface between integrated systems and the biological world. The manipulation of interfaces to facilitate the assembly, reconfiguration, and healing of bio-nano-composite materials is a parallel research theme. Current research activities involve: 1) fundamental studies of the interactions between biological materials and surfaces, 2) development of monolayers that can be programmed with heat, light, or electric fields to switch interfacial interactions leading to the reversible adsorption and desorption of biological species in ”on-chip” environments, and 3) exploitation of active biological species to provide functional interfaces in microfluidic systems (e.g. the use of motor proteins and microtubules to promote the active transport, assembly, and reconfiguration of nanomaterials). Research skills include the synthesis, characterization, and deployment of self-assembled monolayers containing active molecular species. Special CINT capabilities that are available to support research in bioactive interfaces include: 1) the interfacial force microscope (IFM) and other scanning probe systems for probing interfacial interactions, 2) CINT Discovery Platforms that provide on-chip laboratories for studying the adsorption and functionality of bio-materials in microfluidic environments, and 3) a special microfluidic cell designed for studying bioadsorption phenomena using LANL’s neutron scattering capabilities (LANSCE facilities).

Contact: bcbunke@sandia.gov, (505) 284-6892
Thrust: Soft, Biological and Composite Nanomaterials
Location: Core Facility

Andrew M. Dattelbaum
My primary research interests are generally centered around nanostructured silica materials, as well as the preparation of functional self-assembled monolayer systems. I work on a number of projects in these areas with the goals of preparing new materials that are bio-mimetic, optically active, or useful for a variety of sensing applications. In particular, I have worked extensively on the preparation, characterization and functionalization of ordered nanocomposite silica thin films prepared by spin-coating or dip-coating techniques. An integral part of my work includes using self-assembly coupled with synthetic chemistry techniques to functionalize silica materials with reactive binding sites. Current projects include the functionalization of silica materials to immobilize active proteins for characterization studies or sensing applications. Further, projects involving the synthesis of functional silica nanoparticles for various sensing and tracking applications are also ongoing. Other projects include the preparation of self-assembled siloxane surfaces that both target a specific analyte and minimize non-specific bio-interactions. Other self-assembly projects include the controlled formation of supported lipid membrane architectures, which mimic specialized cellular membrane structures, by liposome formation or Langmuir-Blodgett techniques. We have a suite of methods available to characterize all of the above materials, including X-ray diffraction, spectroscopic ellipsometry, absorption and fluorescence spectroscopy, infrared spectroscopy and imaging fluorescence microscopy.

Contact: amdattel@lanl.gov, (505) 665-0142
Thrust: Soft, Biological and Composite Nanomaterials
Location: Gateway Facility

Anatoly Efimov
Primary research interests are in the area of ultrafast nonlinear optics, photonic crystal fibers and devices, femtosecond pulse shaping and coherent control with adaptive feedback. Interests also include nanoplasmonics, fundamentals and applications and active nanophotonic devices. Current research activities are focused on ultrafast optical pulse dynamics in photonic crystal fibers, dynamics and control of solitons and their interaction with continuous waves, supercontinuum and harmonic generation in nanostructured waveguides and soft glass fibers,

visualization of complex nonlinear behaviors with cross-correlation frequency-resolved optical gating (XFROG). Research skills include femtosecond optics, lasers, amplifiers, diagnostics, pulse shaping and its applications to coherent control, general fiber optics, solitons, ultrafast nonlinear processes and their visualization. The primary CINT capabilities utilized include 100-femtosecond tunable telecom-band laser system and continuous wave lasers, custom XFROG setup, custom pulse shaping capabilities, various diagnostics equipment. Future capabilities will include widely tunable 10-femtosecond white light parametric laser system for multispectral time-resolved studies of nanophotonic and nanoplasmonic devices.

Contact: efimov@lanl.gov, (505) 667-5506
Thrust: Nanophotonics and Optical Nanomaterials
Location: Gateway Facility

Amalie Frischknecht
Primary research interests are understanding the structure, phase behavior, and self-assembly of complex fluids and nanocomposites, particularly polymer nanocomposites, polymer melts and solutions, and lipid bilayers. Other interests include the modeling of biopolymers near interfaces and nanoparticles, and the rheology of polymer melts and of suspensions. Current research is focused on the development and use of molecular theory and coarse-grained models to explore the structure and interactions in polymer/nanoparticle blends and thin films and self-assembly in lipid bilayer systems. Molecular theories such as classical density functional theory are quite useful for studying nanoscale systems because they can reach longer time and length scales than atomistic simulations, thus making the nanoscale accessible, and yet can still describe systems on a coarse-grained molecular level. Research skills include the use of classical density functional theory for fluids, molecular dynamics and Monte Carlo simulations, and statistical mechanics. The CINT capabilities utilized include Tramonto (a parallel, classical density functional theory code), LAMMPS (a parallel molecular dynamics code), and various computational clusters.

Contact: alfrisc@sandia.gov, (505) 284-8585
Thrust: Theory and Simulation of Nanoscale Phenomena
Location: Core Facility

Aaron Gin
Primary research interests are in the area of nanostructured photonic and electronic materials, with an emphasis on the fabrication of novel optoelectronic devices. Current research interests focus on the use of electron beam lithography to realize 'top-down' nanometer-scale features in a variety of devices and material systems including Si, III-V compound semiconductors and silica glass. Projects include nanopatterning of diffractive optics, field-effect transistor gates and laser cavities, as well as the development of terahertz quantum cascade lasers and Type II InAs/GaSb infrared detectors. Previous research interests include nanowire and nanopillar device fabrication in III-V material systems, substrate patterning for novel epitaxial material and optoelectronic device testing. Research skills include working knowledge of various material growth techniques and extensive experience in photolithography, electron beam lithography, wet and dry etching, thin film deposition, rapid thermal annealing, wire and die bonding, thermal and electron beam metal deposition, wet chemical surface passivation treatment, polyimide planarization, chemical mechanical polishing (CMP), surface profilimetry, flip chip bonding and wafer dicing. Knowledge of material and device characterization techniques include scanning electron microscopy, atomic force microscopy, x-ray diffraction, photoluminescence, electroluminescence, blackbody, and Fourier transform infrared (FTIR). The primary CINT capabilities utilized include electron beam lithography, scanning electron microscopy, atomic force microscopy and various clean room processing such as photolithography, metal and dielectric deposition and wet and dry etching.

Contact: agin@sandia.gov, (505) 284-1260
Thrust: Nanophotonics and Optical Nanomaterials
Location: Core Facility

Peter Goodwin
Primary research interests are Single-Molecule Spectroscopy (SMS), its application to the study of biomolecular interactions, and the development of SMS-based bioanalytical tools. Ongoing research projects and collaborators

include: Single-molecule fluorescence detection of specific unamplified mRNA transcripts for Leukemia diagnostics. Fluorescence spectroscopy of green fluorescent protein (GFP) variants to elucidate the photophysics of GFP under one- and two-photon excitation. Correlated single-molecule force and fluorescence measurements on GFP variants to explore the relationship between GFP folding stability and fluorescence properties. Evanescent wave scattering readout of polymer tether extension for massively parallel force-extension measurements on single polymer molecules. Single-molecule tracking in 3-dimensions; Single-molecule sorting. Experimental capabilities of possible interest to CINT users: Two-color scanning confocal and flow setups for fluorescence correlation spectroscopy (FCS) and single-molecule fluorescence detection of unamplified nucleic acid sequences. Confocal microscope for one- and two-photon excited single-molecule fluorescence spectroscopy. Capabilities include: time-correlated single-photon counting, FCS, and polarization anisotropy measurements in one or two emission channels. Confocal imaging with single-molecule spectroscopy capabilities will be available in the LANL CINT gateway (Fall 2006).

Contact: pmg@lanl.gov, (505) 665-2506
Thrust: Soft, Biological and Composite Nanomaterials
Location: Gateway Facility

Gary S. Grest
Primary research interests are in computational materials science with emphasis on complex fluids, polymer melts and networks, self-assembled monolayers, and granular materials. Numerical simulations are primarily carried out using LAMMPS, a parallel molecular dynamics code for classical atomistic and coarse grained level simulations. Current research activities are focused on friction and wear between an AFM tip and a surface coated with alkylsilane self-assembled monolayers, spreading of nanodroplets on patterned surfaces, mechanical properties of polymer melts and networks, effect of hydration on polymer adhesion, and flow and packing of granular materials. We are currently developing a new parallel simulation code to model flow and rheology of nanoparticle assemblies in a background media. My primary CINT activities include modeling protein hydrogels, the mechanics of the actin networks and the effect of nanoparticles on the wetting and spreading of liquid drops.

Contact: gsgrest@sandia.gov , (505) 844-3261
Thrust: Theory and Simulation of Nanoscale Phenomena
Location: Core Facility

Jennifer Hollingsworth
Primary research interests are the synthesis, assembly and integration of novel optical and electronic nanoscale materials. Special emphasis is given to developing new synthetic routes to semiconductor quantum dots and nanowires with enhanced functionality for application in optical tag technologies (e.g., bioimaging), optical coatings, light generation, chemical and bio-sensors, solar cells, thermoelectrics, and radiation detection. Useful optical and electronic properties derive from the choice of nanomaterial composition (e.g., PbSe-based quantum dots for near-to-mid-infrared emission), architecture (e.g., core-shell/core-multishell heterostructuring for enhanced emission efficiencies, stability, and reduced cytotoxicity) and the introduction of optically active "impurities" (e.g., lanthanide dopants for ultra-narrow emission signatures). All preparations are conducted in solution at relatively low temperatures (80 - 380ƒC) producing soluble, high-crystalline-quality, processable nanomaterials. The quantum dots and nanowires are compatible with low-temperature assembly and integration approaches utilizing biomolecular templates, amphiphilic polymers, and printing strategies. In addition to standard air-sensitive handling/Schlenk-based synthetic methods, a microwave reactor system and a micro flow reactor system are available for implementing novel synthetic strategies to achieve improved chemical yields, particle size control, new chemical compositions (e.g., alloys, doped nanoparticles), and new architectures (e.g., heterostructured nanowires, covalently linked nanoparticle dimers). Basic structural properties are investigated using a combination of electron microscopies (TEM, STEM, SEM) and powder X-ray diffraction (Rigaku Ultima III with SAXS, DSC, and thin-film attachments). Optical characterizations routinely performed in the synthetic chemistry laboratory include UV-visible-near-IR absorption, fluorescence and photoluminescence excitation spectroscopies.

Contact: jenn@lanl.gov, (505) 665-1246
Thrust: Nanophotonics and Optical Nanomaterials
Location: Gateway Facility

Updated 12-15-09

Julia W. P. Hsu

Primary research interests are in the area of growth and assembly of nanomaterials on surfaces, with emphasis on using organic materials to direct and control inorganic crystal growth. Current research activities include patterned growth of ZnO nanostructures on metals, semiconductors, and transparent conductors, understanding of substrate structural, morphological, and chemical properties on ZnO growth, characterization of optical, electrical, and piezoelectric properties of individual nanostructures, and modeling of the effect of patterning on nucleation density. Additional interests include transport properties at the interface of organic and inorganic materials, novel approaches for patterning materials and for making electrical contacts to organic materials, and surface functioning using small molecules for integration of dissimilar materials. Examples of research activities include fabrication and characterization of metal-molecule-semiconductor diodes, growth of metal organic frameworks on surfaces, characterization of monolayer formation on GaAs surfaces, and improving performance of organic-inorganic hybrid solar cells. Research skills include novel (soft) nanolithography (microcontact printing, micromolding, nanotransfer printing, solution stamping nanolithography, etc.), conducting-tip atomic force microscopy (scanning Kelvin force microscopy, scanning capacitance microscopy, scanning current-voltage microscopy, scanning gate microscopy, piezoelectric force microscopy, etc.), self-assembled monolayer formation, metal-semiconductor transport, and aqueous solution growth of ZnO and related nanostructures. The primary CINT capabilities utilized include novel (soft) nanolithography, surface modification and patterning, crystal growth by solution methods, atomic force microscopy, and transport studies at variable temperatures (4-400K).

Contact: jwhsu@sandia.gov, (505) 284-1173
Thrust: Soft, Biological and Composite Nanomaterials
Location: Core Facility

Han Htoon

Primary research interests are in the area of nanooptics with emphasis on fundamental photophysics, ultrafast carrier dynamics and energy transfer processes of nanoscale materials such as colloidal nanocrystals, quantum dots, quantum wires, and carbon nanotubes. Interests also include spin resolved optical imaging/spectroscopy, chemical imaging of nanoscale materials and their environments, and nanoplasmonics. Current research activities are focused on detection and manipulation of single magnetic spin in magnetic impurity doped, II-VI nanocrystals, and study on fundamental photophysics of semiconducting, single walled carbon nanotubes. Research skills include photoluminescence (PL) and PL excitation spectroscopy of individual nanoscale materials at low temperature and in high magnetic field, nonlinear ultrafast spectroscopy and low temperature near-field scanning optical microscopy/spectroscopy (NSOM). CINT capabilities utilized include optical microscopy, single-molecule fluorescence detection, imaging and spectroscopy techniques, fluorescence, Raman and UV-Vis spectroscopy, femtosecond broadband transient absorption spectroscopy, time-resolved photoluminescence, and the advanced scanning probe facility which is capable of performing NSOM, atomic force, electrostatic force and scanning current-voltage microscopy operations at cryogenic temperature.

Contact: htoon@lanl.gov, (505) 667-9777
Thrust: Nanophotonics and Optical Nanomaterials
Location: Gateway Facility

Jianyu Huang

Primary research interests are in-situ electron microscopy of nanostructured materials. Currently there exists a gap between the microstructure and the corresponding physical property studies of nanostructured materials, i.e. studying the microstructure without knowledge of the related physical properties, or vice versa. We intend to bridge this gap by conducting integrated studies on the microstructure and electrical, mechanical, and thermal properties of individual nanostructures, such as carbon nanotubes, nanowires, and other bulk nanostructured materials. Some specific research topics are: 1) dislocations and other structural defects in carbon nanotubes and their effect on the electrical, mechanical and thermal properties of carbon nanotubes, 2) strength and deformation mechanisms of nanowires; electrical and mechanical coupling of nanowires, 3) in-situ thermal and thermoelectric properties of carbon nanotubes and nanowires, 4) in-situ nano-indentation of bulk nanostructured materials; in-situ TEM of incipient plasticity; deformation mechanisms of nanostructured materials, 5) developing MEMS-based in-situ tensile stressing platforms and MEMS-based in-situ thermal microscopy platforms, 6) structure and properties of InGaAs quantum dots and other semiconducting materials. The CINT TEM laboratory has a state-of-the-art Tecnai F30 field-emission gun transmission electron microscope with a point-to-point resolution of 0.20 nm (at 300 kV) and with electronic imaging obtained with a 4k x 4k CCD camera, as well as scanning capabilities (STEM, including BF, DF and HAADF detection), characteristic elemental x-ray detection with EDS, and energy-filtered imaging (2k x 2k) along with electron energy loss spectroscopy (EELS). We will have Nanofactory TEM-STM, TEM-AFM, and TEM-Nano-indentor platforms enabling simultaneous microstructure and electrical and mechanical property studies of nanostructured materials. We are developing a MEMS TEM-STM platform to do in-situ thermal property studies of nanotubes and nanowires.

Contact: jhuang@sandia.gov, (505) 284-5963
Thrust: Nanoscale Electronics and Mechanics
Location: Core Facility

Dale L. Huber
Research interests are focused on wet chemical methods for the synthesis of nanostructured materials, and the subsequent characterization of these materials. Particular emphasis is in the areas of *in situ* thin film synthesis of polymer monolayers, and the synthesis of nanoparticles. Polymer monolayers are synthesized by free radical polymerization, chain transfer to a surface, as well as a variety of other techniques. Particular interest is in responsive polymers that can alter their surface properties in response to external stimuli. The interaction of these monolayers with biological materials is being explored in earnest. Nanoparticles of a wide variety are regularly synthesized, but those of primary current interest are magnetic particles (iron in particular), titania, and the noble metals. Core-shell particles are also under investigation. Custom synthesis of surfactants is a substantial part of the nanoparticle research, as the surfactants are critical to the quality of particles produced. A variety of tools are utilized to characterize these materials, including: attenuated total reflection IR, reflection-absorption IR, reflection-absorption UV-vis, imaging spectroscopic ellipsometry, contact angle measurements, Transmission electron microscopy, selected area electron diffraction, SQUID magnetometry, NMR, and AFM.

Contact: dlhuber@sandia.gov, (505) 844-9194
Thrust: Soft, Biological and Composite Nanomaterials
Location: Core Facility

Sergei Ivanov
Primary research interests are in the chemistry of electronic and magnetic nanomaterials, with an emphasis on the synthesis, characterization and properties of colloidal semiconductor and metal core-shell nanocomposites. Current research interests focus on colloidal synthesis of core-shell heterocomposites for optical and photovoltaic applications. Research includes core-shell nanocrystals growth mechanisms, structure, optical and electronic properties. Additional research interests include the synthesis and properties of chemically doped colloidal nanostructures as well as the design and synthesis of hybrid colloidal metal/semiconductor nanostructures with new functionalities. Research skills include air-sensitive inorganic, organometallic, and colloidal synthetic chemistry, methods of chemical-physical analysis (NMR, FTIR, single crystal and powder XRD, mass-spectroscopy, UV-Vis and photoluminescence spectroscopy); quantum chemical calculations (ab initio and DFT). The primary CINT capabilities utilized include fully equipped chemical lab, which include two 6-foot fume hoods with vacuum and N 2 atmosphere Schlenk lines, two Ar-atmosphere glove boxes, and t ypical chemical glassware and supplies (e.g., temperature controllers, heating tapes, stir plates, drying ovens, DI water, centrifuge, etc.) Various methods of chemical-physical analysis include FTIR, UV-Vis, photoluminescence, TEM, and SEM available on-site. Access to NMR, XRD, and XRF is also possible.

Contact: ivanov@lanl.gov, (505) 665-4379, (505) 284-7971
Thrust: Nanophotonics and Optical Nanomaterials
Location: Core Facility

Quanxi Jia
Primary research interests are in the area of complex functional materials, with an emphasis on multifunctional nanocomposite metal-oxide films, nanostructured multilayer structures, and their derived novel devices. Current interests are to establish a true materials science triangle of processing, structure, and properties . Research includes

the growth of nanocomposite and nanostructured multilayer metal-oxide films using both pulsed laser deposition (PLD) and polymer-assisted deposition (PAD), the use of strain engineering to tune the physical properties of nanoscale metal-oxide films, and the identification of the fundamental mechanisms of the lattice-strain and size effect on the properties of chemically homogeneous nanoscale metal-oxide films. Examples of metal-oxides include, but not limited to, insulating, dielectric, semiconductive, ferroelectric, ferromagnetic, piezoelectric, multiferroic, metallic, and superconductive materials. Research skills include epitaxial growth of complex metal-oxide films by PLD and PAD, structural and electrical characterization of the materials, and fabrication of their related devices. The primary CINT capabilities utilized include PLD, PAD, electron microscopy, and various other processing and characterization capabilities such as focused ion beam patterning and photolithography, as well as RBS and high resolution x-ray diffraction.

Contact: qxjia@lanl.gov, (505) 667-2716
Thrust: Nanophotonics and Optical Nanomaterials
Location: Gateway Facility

Michael Lilly
Primary research interests are in the area of nanoelectronics, with emphasis on the role of interactions in coupled nanoelectronic structures and 2D bilayers, and coherent electronic effects in nanostructures. Interests also include 2D electron physics, the quantum Hall effects, transport in quantum wires, single photon detectors and quantum computing. Current research activities include tunneling measurements of coupled quantum wires, investigation of the 0.7 structure in single semiconductor quantum wires using transport and fabrication and measurement of electron-hole bilayers for exciton condensation studies. Research skills include cryogenic techniques, semiconductor processing, patterning with electron beam lithography, transport measurements of low dimensional systems and electronic characterization of nanostructures using high magnetic field, low temperature and transport.. The primary CINT capabilities utilized include cryogenic systems (0.02 K to room temperature) with high magnetic field capability (up to 13 T), device fabrication in the clean room, electron beam lithography and development of the Nanosystems Integration Discovery Platform TM.

Contact: mplilly@sandia.gov, (505) 844-4395
Thrust: Nanoscale Electronics and Mechanics
Location: Core Facility

Ting S. (Willie) Luk
Primary research interest is in energy transfer physics of nanomaterials in the vincity of photonic, acoustic (phononic) bandgap materials, and plasmonics. Current research activities are centered around: 1) Using photonic crystals to control radiative processes of nanoparticles such as quantum dots by utilizing the photonic bandedge effect or high Q cavities as part of the development of an active photonic crystal emitter. Another area of interest is using photonic crystals as a negative index metamaterial for imaging and thermal energy harvesting. In addition, we are constantly in the pursuit of new fabrication techniques that can produce low cost, high quality high yield photonic crystals. 2) Another research focus is in the phononic bandgap materials the acoustic counter part of photonic crystals. The interest there is to manipulate and engineer phonon behavior at frequencies from RF ultimately to THz. Phonon control in the THz regime is of particular interest in understanding thermal relaxation processes in nanomaterials. 3) Surface enhance Raman Spectroscopy is the third frontier; photonic and plasmonic crystals can be used as optical antennas with a unique ability to concentrate electromagnetic fields to sub-wavelength scales this allows the unprecedented probing of characteristic molecular dynamics on metallic surfaces.

Contact: tsluk@sandia.gov, 505-844-8931
Thrust: Nanophotonics and Optical Nanomaterials
Location: Core Facility

Jennifer S. Martinez
Primary research interests are in biomaterials synthesis and biosensors, with emphasis on producing and utilizing molecular recognition molecules for the hierarchical assembly of materials. Current research activities are focused on producing nano- and macro-scale biosensors that are reagentfree and field deployable; the use of combinatorial

libraries to synthesize small monodisperse gold and silver nanoclusters; and the study and predictive control of nanoparticle interactions with mammalian cells. Additional research interests include the production of unique phage display libraries for biocompatible materials generation; the study of colligative properties of lipid assemblies produced by molecular recognition; and the production of heterobifunctional ligands for materials assembly. Research skills include characterization of ligand organized lipid assemblies by light scattering, microscopy, and langmuir-blodgett films; natural product structure determination (NMR, MS-MS); chemical conjugation methods; biosensor development; biosynthesis of nanomaterials; and recombinant biology and biochemistry (cloning and protein chemistry). Primary CINT capabilities utilized include large standard molecular biology and biochemistry laboratories for recombinant protein generation; phage display of custom peptide and scFv libraries; peptide-synthesis and characterization; mammalian cell culture and interaction of such with nanoparticles.

Contact: jenm@lanl.gov, (505) 665-0045
Thrust: Soft, Biological and Composite Nanomaterials
Location: Gateway Facility

Amit Misra
Primary research interests are in the area of nanomechanics, with emphasis on fundamental understanding of the mechanical response of nanoscale and nano-composite materials, strain-derived new atomic arrangements at interfaces and novel physical behavior of nanoscale materials. Interests also include nano-engineered multi-functional materials, development of cantilever-based test platforms for nano-mechanical characterization, and mechanics of bio-inspired nanoscale materials. Current research activities are focused on materials systems such as nanolayered composites where the thickness of the individual metal, alloy or ceramic layers are well controlled down to a nanometer, as well as on nanoporous metals and nano-twinned metals. For these materials a broad range of mechanical and physical properties are studied including, but not limited to, residual stresses, strength and fracture, fatigue, creep, thermo-mechanical stability, radiation damage, and electrical and magnetic effects. Research skills include transmission electron microscopy, synthesis of nano-materials using physical vapor deposition, and nanomechanical testing. The primary CINT capabilities utilized include magnetron sputtering, electron beam evaporation, pulsed laser deposition, focused-ion beam (FIB) machining, scanning electron microscopy, transmission electron microscopy, nano-indentation, thin film residual stress measurement, micro-tensile testing, micro-fatigue testing of cantilever samples, and the cantilever Discovery Platform TM.
Contact: amisra@lanl.gov, (505) 667-9860

Location: Gateway Facility

Normand A. Modine
Normand A. Modine is interested in using computational techniques to research energy transfer processes, interfaces and surfaces, and new methodologies for bridging length and time scales. Within the general area of energy transfer processes, Normand is particularly interested in the processes by which electrons tunneling through a surface and excited electronic states captured by defects lose energy to local vibrational modes, as well as, the processes by which the vibrational energy of a nanoscale resonator is dissipated into heat. Normand has considerable experience in calculating the structure and energetics of reconstructed surfaces, and he would like to apply this experience to similar calculations for interfaces and/or surfaces with absorbed organic molecules. Finally, Normand is interested in developing new approaches to bridging length and time scales with emphasis on coupling quantum electronic structure to classical atomistics in order to accurately capture the interplay of local chemistry and collective phenomena. Normand is one of the principle developers of the Socorro electronic structure software, a full featured, open source, massively parallel code for performing Kohn-Sham Density Functional Theory (DFT) calculations. This code can be used to calculate relaxed structures, energetics, transition states, and molecular dynamics trajectories for systems involving up to 1000 atoms, as well as providing electronic densities and wavefunctions. In addition, Normand has developed a hybrid quantum/classical code in which a region represented with the DFT is embedded within a system represented using classical potentials.

*Contact:*namodin@sandia.gov, (505) 844-8412
Thrust: Theory and Simulation of Nanoscale Phenomena
Location: Core Facility

Gabriel Montano
Primary research interests are in the area of bio-inspired and bio-integrated materials with an emphasis on design and characterization of interactions at the bio-synthetic interface. Along with an interdisciplinary research team at LANL, we are currently investigating biological responses to nanomaterials employing a variety of approaches and techniques ranging from cell and molecular biology techniques to bio-inspired materials approaches. Current investigations from the biomaterials perspective are looking at mechanistic responses of nanomaterials interacting with biological structures including lipid membranes and model protein systems. Optical and scanning probe microscopies as well as various vibrational spectroscopies are used to mechanistically determine effects such as cytotoxicity due to nanomaterial incorporation observed by cellular studies. Other research focuses on creating bio-inspired and bio-integrated assemblies. Various functionalized synthetic materials such as fullerenes and conjugated polymers are assembled along with lipid membranes to mimic biological functions such as long-lived charge separation and also create interactions at the bio-synthetic interface. Self-assembly and directed assembly approaches such as silane chemistry, vapor deposition, polyelectrolyte interactions and thin-film deposition and patterning are used to create assemblies and various types of microscopy and spectroscopy are used for characterization. The primary CINT capabilities used in the above research include self-assembled monolayer formation, liposome and lipid bilayer formation via extrusion, in situ scanning probe microscopy including electrochemical AFM, optical microscopies, various steady-state and time-resolved spectroscopies and various surface modification and characterization techniques including small-scale patterning and ellipsometry.

Contact: gbmon@lanl.gov, (505) 667-6776, (505) 284-8236
Thrust: Soft, Biological and Composite Nanomaterials
Location: Core Facility

Tom Picraux
Primary research interests are in the area of nanostructured electronic materials, with an emphasis on the synthesis, characterization and properties of semiconducting nanowires, as well as their integration into microscale systems. Current research interests focus on CVD Vapor-Liquid-Solid (VLS) growth of silicon and germanium nanowires and Si/Ge linear and core-shell nanowire heterostructures. Research includes nanowire growth mechanisms, kinetics, structure, strain distributions, chemical doping, optical and electronic properties, bandstructure engineering, and the assembly of nanowires into electrode arrays. Additional research interests include the synthesis and properties of nanoporous thin films such as Pt and Au formed by electrochemical dealloying, and the formation of photoswitchable superhydrophobic surfaces by functionalizing nanowires or other structured surfaces with monolayer coatings containing photochromic molecules. Research skills include CVD VLS nanowire synthesis, thin film deposition, Rutherford backscattering spectrometry (RBS) and ion channeling, surface modification, and a variety of electronic materials processing, structural, and property characterization techniques. The primary CINT capabilities utilized include VLS Si/Ge nanowire synthesis by CVD, vapor deposition, RBS, scanning electron microscopy, interfacial force microscopy, the Electrical Transport Discovery Platform TM, and various processing capabilities such as metal and dielectric deposition, plasma etch, focused ion beam patterning, photolithography, and wet processing.

Contact: picraux@lanl.gov, (505) 665-8554
Thrust: Nanoscale Electronics and Mechanics
Location: Gateway Facility

Rohit Prasankumar
My primary research interests focus on the measurement of ultrafast dynamics in complex functional materials, particularly in semiconductor nanostructures and correlated electron materials. Additional interests are in the area of nanophotonics, in particular the development and characterization of metamaterials and surface plasmon-based devices. Current research focuses on ultrafast spectroscopy in the mid-to-far-infrared frequency range, where the dynamical properties of important spectral features such as optical phonon resonances, the superconducting gap in high-Tc superconductors, and energy level spacings and intersubband transitions in semiconductor nanostructures can be studied. In addition, the use of near field scanning optical microscopy to study complex materials is expected to provide much insight into issues including nanoscale phase separation in transition metal oxides and localized electric fields in nanophotonic devices. Finally, in collaboration with CINT users, use of the Optical and Transport Discovery PlatformTM to integrate ultrafast optical measurements with other CINT capabilities promises to yield

new perspectives on fundamental phenomena in nanoscale materials and devices. Research skills include ultrafast optical spectroscopy in the spectral range from the visible to far-infrared, terahertz time-domain spectroscopy (THz-TDS), and near-field scanning optical microscopy (NSOM). CINT capabilities utilized in this research include the Optical and Transport Discovery Platform TM, NSOM (available fall 2006), a visible sub-10 fs pulsed laser system (available summer 2006), THz-TDS, high sensitivity femtosecond transient absorption spectroscopy, and optical-pump mid/far-infrared-probe spectroscopy.

Contact: rpprasan@lanl.gov, (505) 284-7966
Thrust: Nanophotonics and Optical Nanomaterials
Location: Core Facility

John Reno
Primary research interests are in the area of nanostructured electronic materials, with an emphasis on the synthesis of AlGaAs based materials. Current research interests focus on intersubband transitions and high mobility heterostructures. Research includes quantum cascade lasers (QCL) in the THz and IR range, quantum well infrared photodetectors (QWIP), and high mobility materials for quantum transport studies. The primary CINT capabilities utilized include molecular beam epitaxy (MBE) calibration, growth, and materials characterization of AlGaAs based materials.

Contact: jlreno@sandia.gov , (505) 665-8554
Thrust: Nanoscale Electronics and Mechanics
Location: Core Facility

Andrew P. Shreve
Primary research interests are in the area of soft and biological materials, with an emphasis on the use of spectroscopic techniques for characterization of material structure, dynamics and function. Specific areas of expertise include the applications of spectroscopic techniques to the study of electron and energy transfer processes in biology, chemistry and nanoscale materials science. Techniques used include electronic and vibrational spectroscopies and time-resolved spectroscopies. Interests in this area also include the development and use of spectro-electrochemical methods. A related area of interest is the development of spectroscopic and optical imaging methods, including experimental and theoretical aspects of time-resolved and nonlinear spectroscopies, ultrasensitive imaging methods, surface specific spectroscopies and Raman spectroscopies. Other scientific interests include the development and applications of thin-film nanostructured self-assembled and biomimetic membrane architectures. This class of materials includes substrate-supported phospholipid membranes, Langmuir-Blodgett assemblies, and polyelectrolyte (including protein) assemblies. The development of such materials with electronic or optical responses, and the characterization of those responses using optical spectroscopies and imaging is of interest. Also, such materials are applicable to many biosensing strategies and the development biosensors and molecular transduction strategies is of interest. Primary CINT capabilities used include optical, Raman and infrared spectroscopies, optical imaging, fluorescence microscopy, ellipsometry, electrochemistry and spectroelectrochemistry, Langmuir-Blodgett techniques, preparation and characterization of protein and membrane samples, and thin-film self-assembly methods.

Contact: shreve@lanl.gov, (505) 667-6933
Thrust: Soft, Biological and Composite Nanomaterials
Location: Gateway Facility

Mark Stevens
Primary research interests are in the theory of nano-bio interfaces, with emphasis on fundamental understanding of the self-assembly and basic dynamical processes. Current research involves soft materials including biomembranes, polyelectrolytes, self-assembled monolayers, proteins, and polymer networks. Using both atomistic and coarse-grained models, the systems are studied using molecular dynamics and/or Monte Carlo simulations. Recent coarse-grained simulations of lipid systems reach the time scale (milliseconds) at which collective biomolecular dynamics yields a functional (biological) process. Other research interests include the theory of nanomechanics and complex functional materials. Modeling of adhesion and friction between various self-assembled monolayers has been a

research focus, and now we are explicitly modeling tip interactions. The interface between soft and hard materials is another interest, especially for polymers at silica surfaces. Research skills include atomistic and coarse-grained modeling, molecular dynamics and Monte Carlo simulations. The primary CINT capability includes the LAMMPS parallel molecular dynamics code.

Contact: msteve@sandia.gov, (505) 844-1937
Thrust: Theory and Simulation of Nanoscale Phenomena
Location: Core Facility

John P. Sullivan
Primary research interests are in the area of nanomechanics, with emphasis on the creation of micro- and nanomechanical structures for fundamental understanding of phenomena associated with the motion, displacement, or vibration of structures. Specific interests include the creation of MEMS and NEMS structures for studies of the elastic properties, fracture, and fatigue of materials; the creation and measurement of micro- & nanomechanical resonators to understand the size-, geometry-, material-, surface-, and temperature-dependence of mechanical dissipation in structures; studies of chemical, biological, or environmental sensing using mechanical structures; studies of emergent or complex behavior in large arrays of coupled mechanical elements; the development of structures for the study of phonon transport in geometrically-confined systems; and the development of new mechanical structures to support novel scanning probe microscopy experiments. Recent research activities have focused on the use of torsional and flexural MEMS resonators to measure the activation energy for defect relaxation processes in amorphous and crystalline diamond thin films and the creation of large arrays of coupled mechanical oscillators to understand emergent behavior in low-dimensional systems. Research skills include semiconductor processing and MEMS and NEMS synthesis, mechanical and electrical characterization of materials, and AFM and STM in ultra-high vacuum (UHV). The primary CINT capabilities utilized include clean room semiconductor processing (lithography, metal and dielectric deposition, dry etching, surface micromachining), laser light scattering and interferometry for MEMS resonator characterization, stress and elastic property measurement using cantilever deflection or resonator structures, UHV AFM and STM, and the Cantilever Array Discovery Platform TM.

Contact: jpsulli@sandia.gov, (505) 845-9496
Thrust: Nanoscale Electronics and Mechanics
Location: Core Facility

Brian Swartzentruber
Primary research interests are in the area of kinetics and thermodynamics of nanoscale structures, bridging length scales from atoms to microns, with an emphasis on developing a fundamental understanding of mass transport processes and the stability of nanostructures. Current research activities focus on the determination of atom diffusion processes and their implications for the growth and mobility of larger structures. Examples include the initial stages of nucleation and growth of Ge/Si alloy structures and their pathway to 3-d quantum dot formation, and the atomic diffusion of Pb and Pd atoms in the copper alloy surface leading to a rich variety of concentration-dependent self-assembled surface structures on the nanometer length scale. Additional research activities include developing novel implementations of scanning-probe-like instruments for direct and precise nanomanipulation for top-down construction of unique nanostructures, for 3d-electronics, sensor, and 'NEMS' applications. Primary CINT capabilities include: 1) Ultra-high-vacuum variable-temperature STM [RHK]. 2) Atomic force microscope (AFM) [Veeco] for contact, non-contact, lateral force, magnetic force, tapping mode, lift mode, and electric force microscopy in ambient and liquid environments. Tunneling and conductive AFM, and scanning capacitance modules are currently available. Four-point probe module will be added later. 3) Versatile, custom, variable-temperature STM with atom-tracking capability for user defined applications. Capabilities in collaboration with CINT/SNL Gateway scientists include low-energy electron microscopy and interfacial force microscopy.

Contact: bsswart@sandia.gov, (505) 844-6393
Thrust: Nanoscale Electronics and Mechanics
Location: Core Facility

Updated 12-15-09

Sergei Tretiak
Primary research interests are in the area of theoretical chemical physics, with an emphasis on electronic structure and spectroscopy of organic and inorganic electronic nano-materials. Current research interests focus on theoretical studies of excited states and optical responses of photoactive organic and inorganic nano-materials such as large organic molecules, biological complexes and semiconductor nano-particles. All electronic processes in these systems are governed by strong electronic correlations and coupling of electrons to molecular structure. We develop quantum chemical approaches for efficient and accurate modeling of electronic structure, dynamics, charge and energy transfer in large molecular systems and apply these methods to different materials such as conjugated polymers, dendrimers, carbon nanotubes, biological light harvesting systems, donor-acceptor complexes, and semiconductor quantum dots. The results of the calculations are then used for modeling of linear (absorption and emission) and nonlinear (including ultrafast frequency and time-resolved spectroscopic probes) optical responses to model experimental data and to understand underlying dynamical photo-physical, photo-chemical and relaxation processes. Research skills include various solid state and quantum chemical theoretical techniques such as density functional theory (DFT) and time-dependent DFT (TDDFT); semiempirical methods; classical, quantum and nonadiabatic molecular dynamics; theoretical nonlinear spectroscopy. Numerical simulations utilize a number of commercial and home-made codes as well as analytical modeling.

Contact: serg@lanl.gov, (505) 667-8351
Thrust: Theory and Simulation of Nanoscale Phenomena
Location: Gateway Facility

Stuart Trugman
Primary research interests are in the area of theoretical dynamics of quantum systems, including confined geometries and response to ultrafast optical, infrared, and terahertz probes. Current research activities include calculating the ground state, excited states, and dynamics far from equilibrium of coupled quantum systems, including electrons and excitons coupled to quantum lattice (phonon) degrees of freedom. One aspect is the calculation in real time and real space of how a polaron quasiparticle forms from a bare electron after it is photoinjected or tunnels into a material with electron-phonon coupling. For this problem, it is important that the phonons are treated quantum mechanically. Spin, charge, orbital, and lattice degrees of freedom can be included. Another aspect is the computation of inelastic electron tunneling spectra. Research includes calculating the response of correlated systems, including ferromagnetic and CMR (colossal magnetoresistance), superconducting, and heavy fermion systems to ultrafast optical, infrared, and terahertz probes; this work is closely coupled to experiments. Techniques employed include analytic approaches, Lanczos exact diagonalization of model Hamiltonians in large variational many-body Hilbert spaces, and numerical integration of the time-dependent Schrodinger equation in these Hilbert spaces.

Contact: sat@lanl.gov, (505) 665-1167
Thrust: Theory and Simulation of Nanoscale Phenomena
Location: Gateway Facility

Jim Werner
Primary research interests are in optical microscopy, laser spectroscopy, instrument development, and protein dynamics. Ongoing research projects include the design and construction of microscopic instrumentation for 3-D tracking of individual fluorophores, wide-field single molecule fluorescence imaging studies of protein-ligand association, sorting single molecules in microfluidic environments, and optical trapping and manipulation of particles. Experimental capabilities of possible interest to CINT users: Wide field single molecule fluorescence microscopy via total internal reflection excitation, two photon fluorescence microscopy, fluorescence correlation spectroscopy.

Contact: jwerner@lanl.gov, (505) 667-8842
Thrust: Soft, Biological and Composite Nanomaterials
Location: Gateway Facility

Updated 12-15-09

CINT Distinguished Affiliate Scientists

C. Jeffery Brinker
Our work combines inorganic and hybrid (organic/inorganic) solution-based synthesis with molecular self-assembly to arrive at porous and composite nanostructured films and particles by simple evaporative procedures. Starting with homogeneous solutions of amphiphilic surfactants, lipids, or block copolymers, solvent evaporation drives the self-assembly of micelles and further self-organization into periodic mesophases, serving to organize added hydrophilic inorganic and/or hydrophobic organic precursors. Using such solutions as 'self-assembling inks', we print these periodic nanostructures onto arbitrary surfaces whose nano- micro- and macro-structures can be defined further with light. Replacing standard surfactant micelles with monosized nanocrystal micelles, we use evaporation-induced self-assembly to develop robust, patternable 3D arrays of metallic, semi-conductor or magnetic nanocrystals and to integrate them into devices or platforms, where they can be interrogated electronically, optically, or magnetically. Recently we discovered the ability of living cells to organize extended nanostructures and nano-objects in a manner that creates a unique, highly biocompatible nano/bio interface, mimicking the extra-cellular matrix. Using printing and patterning techniques, we can integrate cells into platforms needed for electronic, optical, and spectroscopic interrogation. Capabilities include self-assembly and directed assembly techniques, lithographic definition and patterning of nano-structured films, thermal and plasma-assisted atomic layer deposition, and sol-gel chemistry.
Contact: cjbrink@sandia.gov, (505) 272-7627
Location: Sandia National Laboratories

Michael Nastasi
Primary research interests are in the area of nanomechanics and nanostructured functional materials with an emphasis on synthesis, modeling, theory, and experiment. The goal of this work is to develop a fundamental understanding of how stresses evolve from atoms residing at surfaces and interfaces in nanostructured materials, how these stresses promote the evolution of new atomic arrangements, and how these stresses and new structures give rise to unique and novel mechanical, electronic, and magnetic properties not seen in bulk materials. Current research interests include studying the size and stress effects on the fatigue properties of ferroelectric materials, using molecular dynamics to study the stability and mechanical properties nanowires, using surface modification techniques to improve the photovoltaic behavior of nanoscale materials, and synthesizing and modifying nanostructured materials and through ion implantation and ion irradiation. Research skills include the synthesis of nano-materials using physical vapor deposition, sol-gel methods, and ion implantation, ion beam analysis (IBA) techniques such as Rutherford backscattering spectrometry, ion channeling, elastic recoil and nuclear reaction analysis, and nanomechanical testing. The primary CINT capabilities utilized include ion implantation, magnetron sputtering, electron beam evaporation, pulsed laser deposition, focused-ion beam (FIB) machining, nano-indentation, thin film residual stress measurement, and the Cantilever Discovery Platform TM
Contact: nasty@lanl.gov, (505) 667-7007
Location: Los Alamos National Laboratory

Darryl Smith
Primary research interests are in the area of condensed matter theory with emphasis on electronic/optical materials and electrical /electro-optic devices fabricated from these materials. Specific interests include semiconductor heterostructures and nanostructures, and the electronic and optical properties of conjugated organic materials. Current research activities are focused on spin physics in semiconductors, electronic properties of disordered organic semiconductors, spin noise spectroscopy, radiation detectors, and organic semiconductor based photovoltaic and light emitting structures. Capabilities include electronic structure calculations, electrical transport and optical property calculations.
Contact: dsmith@lanl.gov, (505) 667-2056
Location: Los Alamos National Laboratory

Antoinette (Toni) Taylor
Primary research interests are in the area of nanophotonics and complex functional nanomaterials, with an emphasis on optical interactions with nanomaterials and the development of novel optics-based techniques to study nanoscale phenomena. Current research activities are focused on ultrafast dynamics of complex materials on the nanoscale,

including spin-charge-lattice interactions in complex nanoscale materials, nonlinear optical effects in microstructured fibers, the ultrafast, nanoscale dynamics of phase transitions in solids, the development of terahertz spectroscopy for the investigation of nanoscale phenomena, the application of coherent control techniques ton condensed phase, and in particular, nanoscale systems, and the development of spatially and temporally local probes for nanoscience applications. Research skills include a background in optical interactions with condensed matter systems, spectroscopic techniques, both conventional and ultrafast, nonlinear optics, and nanoscale scanned probes. The primary CINT capabilities utilized include optical spectroscopy (Raman, infrared, uv-vis, fluorescence spectroscopy, ellipsometry), ultrafast spectroscopies (ultrafast transient absorption, terahertz spectroscopy, ultrafast STM, terahertz NSOM, coherent spectroscopies, frequency-resolved optical gating), nanoscale scanned probes (STM, NSOM) and the optics, transport and photoconductivity Discovery Platform TM.
Contact: ttaylor@lanl.gov, (505) 665-0030
Location: Los Alamos National Laboratory